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CRITICAL TEMPERATURE OF THE SUPERFLUID TRANSITION IN FERMI-SYSTEM AT AN ARBITRARY PAIR POTENTIAL

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A method for calculation of the critical temperature of transition of a many-particle Fermi system into a superfluid or a superconducting state at an arbitrary pair potential of the interparticle interaction is proposed. An original homogeneous integral equation, that determines the critical temperature, is transformed into a homogeneous integral equation with a symmetric kernel that enables application of a general theory of integral equations for calculation. Examples are given of calculation of the superconducting transition critical temperature for the BCS potential with the Coulomb repulsion and the critical temperature of the superfluid transition of liquid helium-3 into *p*-wave pairing state for the Morse potential.

KEY WORDS: critical temperature, superconductivity, superfluidity, pair potential, homogeneous integral equation, characteristic number

КРИТИЧНА ТЕМПЕРАТУРА ПЕРЕХОДУ ФЕРМІ-СИСТЕМИ В НАДПЛИННИЙ СТАН ПРИ ДОВІЛЬНОМУ ПАРНОМУ ПОТЕНЦІАЛІ

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Запропоновано метод розрахунку критичної температури переходу багаточастинкової фермі-системи в надплинний або надпровідний стан при довільному парному потенціалі міжчастинкової взаємодії. Вихідне однорідне інтегральне рівняння, що визначає критичну температуру, перетворюється в однорідне інтегральне рівняння з симетричним ядром, що дозволяє застосувати для розрахунку загальну теорію інтегральних рівнянь. Наведені приклади розрахунку критичної температури надпровідного переходу для потенціалу БКШ з кулонівським відштовхуванням та температури переходу гелія-3 в надплинний стан з *p*-спарюванням для потенціалу Морзе.

КЛЮЧОВІ СЛОВА: критична температура, надпровідність, надплинність, парний потенціал, однорідне інтегральне рівняння, характеристичне число

КРИТИЧЕСКАЯ ТЕМПЕРАТУРА ПЕРЕХОДА ФЕРМИ-СИСТЕМЫ В СВЕРХТЕКУЧЕЕ СОСТОЯНИЕ ПРИ ПРОИЗВОЛЬНОМ ПАРНОМ ПОТЕНЦИАЛЕ

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Предложен метод расчета критической температуры перехода многочастинковой ферми-системы в сверхтекучее или сверхпроводящее состояние при произвольном парном потенциале межчастинчного взаимодействия. Исходное однородное интегральное уравнение, определяющее критическую температуру, преобразуется в однородное интегральное уравнение с симметричным ядром, что позволяет применить для расчета общую теорию интегральных уравнений. Приведены примеры расчета критической температуры сверхпроводящего перехода для потенциала БКШ с кулоновским отталкиванием и температуры перехода гелия-3 в сверхтекучее состояние с *p*-спариванием для потенциала Морзе.

КЛЮЧЕВЫЕ СЛОВА: критическая температура, сверхпроводимость, сверхтекучесть, парный потенциал, однородное интегральное уравнение, характеристическое число

Calculation of the critical temperature of a superfluid or superconducting transition in a Fermi system is a central issue in the theory of superfluid Fermi systems. The importance of this problem has especially risen after the discovery of high-temperature superconductivity [1,2]. In calculation of the critical temperature in the theory of conventional superconductivity [3-5], it is assumed that the interaction between the electrons exists only in a narrow energy range of the order of the Debye energy near the Fermi surface. This allows one to approximate the interelectron interaction potential by a constant. But such approximation becomes fairly rough to account for the influence of the Coulomb interaction[5-7], because in this case the region of interaction is not confined by a narrow energy range. The validity of approximations, employed in calculation of the critical temperature in conventional superconductors, is broken in many cases in high-temperature superconductors. Of special interest is calculation of the transition critical temperature in superconductors with overlapping conduction bands [6-8], because such a model can be used for a theoretical description of superconductivity both in the transition metals and high-temperature superconductors. A detailed analysis of calculations of the superconducting transition critical temperature in different systems is given in the book [9]. It is noted therein that the solving of an integral equation determining the critical temperature for in the least bit complex

interaction “constitutes a well-known problem”.

Taking into account of interparticle interaction only in a narrow range near the Fermi energy in calculation of the temperature of transition of ^3He into the superfluid phase [10] is also, generally speaking, inconsistent. In particular, apparently this is responsible for a difference of some orders of magnitude in theoretical estimations of the ^3He critical temperature in papers of different authors [11,12]. Besides that, the reason of such large discrepancies is connected with sensitivity of the calculated temperature to a choice of parameters of the interparticle interaction potential.

The aim of this paper is to develop a consistent method for calculation of the critical temperature of transition of a many-particle Fermi system into a superfluid or a superconducting state at an arbitrary pair potential of the interparticle interaction. The essence of the proposed method consists in transition to a study of a homogeneous integral equation with a symmetric kernel that enables application of the known results of the theory of integral equations. In principle, the proposed method enables to calculate numerically the critical temperature for an arbitrary interparticle interaction potential with a prescribed accuracy. As examples of use of the proposed method, the critical temperature in the BCS model with a finite ratio of the Debye energy to the Fermi energy is calculated and the influence of the Coulomb repulsion is taken into account. It is shown that the formula for the critical temperature [5,13] in the presence of the Coulomb interaction, obtained earlier by means of an approximate consideration, is exact within the framework of the selected model. The critical temperature of the superfluid transition of liquid ^3He into p -wave pairing state for the Morse potential is calculated and its strong dependence on the value of one of parameters of this potential is shown. At reasonable choice of parameters of the potential, the calculated critical temperature is close to the experimentally observable one.

TRANSFORMATION OF THE EQUATION FOR THE CRITICAL TEMPERATURE TO A HOMOGENEOUS INTEGRAL EQUATION WITH A SYMMETRIC KERNEL

The critical temperature T_C of transition into a superfluid or a superconducting state of a Fermi system is found from the linearized equation for the order parameter $\Delta_{\mathbf{k}}$ [13]:

$$\Delta_{\mathbf{k}} = -\frac{1}{V} \sum_{\mathbf{k}'} U_{\mathbf{k}-\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2\xi_{\mathbf{k}'}} \operatorname{th} \frac{\xi_{\mathbf{k}'}}{2T_C}, \quad (1)$$

where \mathbf{k} is the wave vector, $\xi_k = \hbar^2 k^2 / 2m_* - \mu$, μ is the chemical potential, m_* is the effective mass. Fourier component of the interaction potential has the form

$$U_{\mathbf{k}} = \int d\mathbf{r} U(\mathbf{r}) e^{-i\mathbf{k}\mathbf{r}}, \quad (2)$$

where $U(\mathbf{r})$ is a potential energy of the interparticle interaction. We will consider an isotropic system, and expand the order parameter and the Fourier component of the potential in spherical functions

$$\Delta_{\mathbf{k}} = \sqrt{4\pi} \sum_{l=0}^{\infty} \sum_{m=-l}^l \Delta_{lm}(k) Y_{lm}(\Omega), \quad (3)$$

$$U_{\mathbf{k}-\mathbf{k}'} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^l U_l(k, k') Y_{lm}(\Omega) Y_{lm}^*(\Omega'). \quad (4)$$

Supposing that the potential depends only on a distance $U(\mathbf{r}) = U(r)$, we find for a component of the potential

$$U_l(k, k') = 4\pi \int_0^\infty dr r^2 U(r) j_l(kr) j_l(k'r), \quad (5)$$

$j_l(x) = \sqrt{\frac{\pi}{2x}} J_{l+\frac{1}{2}}(x)$ are Bessel spherical functions. In the case of the singlet pairing, when $\Delta_{\mathbf{k}} = \Delta_{-\mathbf{k}}$, in the expansion (3) only components with even l remain, and for the triplet pairing, when $\Delta_{\mathbf{k}} = -\Delta_{-\mathbf{k}}$, only components with odd l . In an anisotropic medium, for example in a crystal, the expansion of the order parameter and the potential should be made in basis functions of the irreducible representations of a symmetry group of a crystal[14].

Equation (1) decomposes into equations for the separate components of expansions (3), (4) with different l for the order parameter and the potential, which after the transition in (1) from summation to integration acquire the form

$$\Delta_l(k) = -\frac{1}{(2\pi)^2} \int_0^\infty U_l(k, k') F(k'; T_C) \Delta_l(k') k'^2 dk', \quad (6)$$

where $\Delta_l(k) \equiv \sum_{m=-l}^l a_{lm} \Delta_{lm}(k)$, a_{lm} are arbitrary coefficients, because the transition temperature does not depend on the index m . In (6) the designation is introduced

$$F(k) \equiv F(k; T_C) \equiv \frac{1}{\xi_k} \operatorname{th} \frac{\xi_k}{2T_C}. \quad (7)$$

Thus, calculation of the critical temperature comes to finding values of the parameter T_c , at which the homogeneous integral equation

$$\Delta(k) = \int_0^\infty R(k, k') \Delta(k') dk' \quad (8)$$

has different from zero solutions. The kernel of this integral equation

$$R(k, k') = -\frac{1}{(2\pi)^2} U(k, k') F(k'; T_c) k'^2, \quad (9)$$

is, obviously, unsymmetrical $R_l(k, k') \neq R_l(k', k)$. The index l of the order parameter and the potential here and in what follows is omitted.

For subsequent analysis it is convenient to go over to an integral equation with a symmetric kernel, that will allow us to use general results of the theory of integral equations. For this purpose we multiply equation (6) by $k\sqrt{F(k)}$ and define the function $\Phi(k) \equiv k\sqrt{F(k)}\Delta(k)$. As a result we come to the homogeneous integral equation

$$\Phi(k) = \int_0^\infty K(k, k'; T_c) \Phi(k') dk', \quad (10)$$

with the symmetric real kernel

$$K(k, k'; T_c) \equiv K(k, k') = K(k', k) = -\frac{kk'}{(2\pi)^2} U(k, k') \sqrt{F(k)F(k')}. \quad (11)$$

As opposed to the Fredholm homogeneous integral equation of the second kind [15]

$$\varphi(x) = \lambda \int_a^b K(x, t) \varphi(t) dt, \quad (12)$$

in equation (10) a parameter, which role is played by the critical temperature here, enters not as a factor before the integral, but is incorporated in a complicated manner into the kernel of the integral equation $K(k, k'; T_c)$.

Note that the order parameter $\Delta(k)$ is, generally speaking, complex, so that it and the above defined function can be presented in the form $\Delta(k) = \Delta'(k) + i\Delta''(k)$ and $\Phi(k) = \Phi'(k) + i\Phi''(k)$. Because of the kernel (11) being real, identical integral equations come out for the real and the imaginary parts of the function $\Phi(k)$. Therefore, in what follows we consider this function real.

Despite the fact that equation (10) is not of the Fredholm form, finding of the critical temperature can be reduced to finding of characteristic numbers λ of the equation of type (12). To this end, let's consider the auxiliary equation

$$\Phi(k) = \lambda(T) \int_0^\infty K(k, k'; T) \Phi(k') dk'. \quad (13)$$

The kernel of this equation depends on the parameter T , which in our case has the meaning of temperature. Characteristic numbers of equation (13) $\lambda_i(T)$ (several numbers can exist) are functions of temperature. Equation (13) coincide with equation (10) in the case when at some temperature one of characteristic numbers appears to be equal to unity, so that the critical temperature has to satisfy the condition

$$\lambda_i(T_c) = 1. \quad (14)$$

From here on assuming eigenfunctions to be normed by the condition $\int_0^\infty \Phi^2(k) dk = 1$, we get

$$\lambda(T) = \left[\int_0^\infty \Phi(k) K(k, k'; T) \Phi(k') dk dk' \right]^{-1}. \quad (15)$$

Transition to a superfluid state is possible only for such potentials at which equation (13) has positive characteristic numbers. From equation (15) and the form of function (7), it follows that characteristic numbers are large at high temperatures and fall off with decreasing temperature. A phase transition takes place when condition (14) becomes satisfied for one of numbers. If for a given potential condition (14) is not satisfied at any temperature, then a phase transition is not possible. Dependence of the characteristic number on temperature for the potential of the BCS type (20) is shown in figure 1. Qualitatively, dependence of absolute values of characteristic numbers on temperature has a similar form as well for arbitrary potentials.

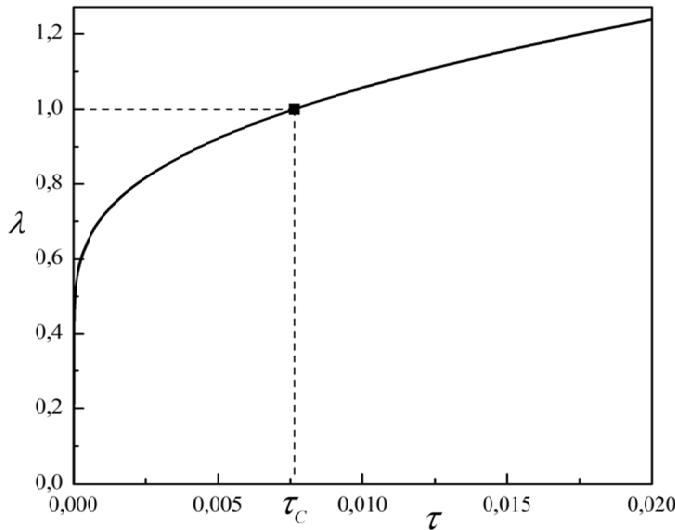


Fig. 1. Dependence of the characteristic number on temperature in the BCS model

$\lambda(\tau) = \left(\frac{g}{2} \int_{-1/\tau}^{1/\tau} dy \frac{1}{y} \operatorname{th} \frac{y}{2} \right)^{-1}, \quad \tau \equiv \frac{T}{\varepsilon_D}, \quad g = 0, 2. \text{ The mark } \blacksquare \text{ designates the point, corresponding to transition to a superfluid state: } \lambda(\tau_c) = 1.$

CRITICAL TEMPERATURE FOR SEPARABLE POTENTIALS

Characteristic numbers of the integral equation (13) can easily be found if, for instance, its kernel can be represented as a product of the two same factors

$$K(k, k') = \nu K(k) K(k'), \quad (16)$$

where $\nu = \pm 1$. Such a representation takes place for potentials of the special form $U(k, k') = -\nu U(k) U(k')$, called separable potentials. In this case

$$K(k) = \frac{k}{2\pi} U(k) \sqrt{F(k)} \quad (17)$$

and the integral equation has the single characteristic number

$$\lambda(T) = \nu \left[\int_0^{\infty} K^2(k) dk \right]^{-1}. \quad (18)$$

This number is positive if $\nu = +1$. In the opposite case the characteristic number is negative and a phase transition is absent. Condition (14) leads to the equation determining the critical temperature for the case of the separable potentials

$$\frac{1}{(2\pi)^2} \int_0^{\infty} U^2(k) F(k; T_c) k^2 dk = 1. \quad (19)$$

Note that the separable model potentials are widely used, for instance, in the theory of the nucleus [16].

The matrix element of the interaction potential in the BCS model can be represented as

$$U(k, k') = -U_0 \psi(k) \psi(k'), \quad (20)$$

where $\psi(k) = \theta(k - k_F - \Delta k) - \theta(k - k_F + \Delta k)$, and $k_F = (3\pi^2 n)^{1/3}$ is the Fermi wave number, n is the electron density, $\theta(k)$ is the unit step function, $U_0 > 0$. The width of the shell nearby the Fermi surface, in which fermions interact, is determined by the Debye frequency ω_D , so that $\Delta k = m_* \omega_D / \hbar k_F$. As seen, the BCS potential is separable, with $\nu = 1$ and $U(k) = \sqrt{U_0} \psi(k)$, and therefore the integral equation (13) has the single characteristic number. In this case equation (19) can be represented in a standard for the BCS theory [3-5] form

$$\frac{U_0}{(2\pi)^2} \int_{k_F - \Delta k}^{k_F + \Delta k} \frac{k^2}{\xi_k} \operatorname{th} \left(\frac{\xi_k}{2T_c} \right) dk = 1. \quad (21)$$

In calculation of the transition temperature into a superconducting state one needs, generally, account for the two energy parameters characterizing a system, namely the Debye energy $\varepsilon_D = \hbar \omega_D$ and the Fermi energy $\varepsilon_F = \hbar^2 k_F^2 / 2m_*$.

In conventional superconductors the Fermi energy is by two orders higher than the Debye energy, so that $\varepsilon_F \gg \varepsilon_D$. In some cases, for instance in high-temperature superconductors [1,2], this strong inequality can be violated. In this connection, let's make calculation of the critical temperature, not assuming the ratio $\Gamma \equiv \varepsilon_D/\varepsilon_F$ to be small, so that equation (21) can be written in the form

$$\frac{U_0 N_F}{2} \int_{-\varepsilon_D/T_C}^{\varepsilon_D/T_C} \sqrt{1 + \frac{T_C}{\varepsilon_F} y} \cdot \operatorname{th}\left(\frac{y}{2}\right) \frac{dy}{y} = 1, \quad (22)$$

$N_F = m_* k_F / 2\pi^2 \hbar^2$ is the density of states at the Fermi surface. Usually, assuming that $\Gamma \ll 1$, the square root in formula (22) is assumed to be unity. In addition, in further calculation in the BCS theory it is assumed that $\varepsilon_D \gg T_C$.

This condition is also violated in the HTSC. A standard BCS formula for the superconducting transition temperature, calculated under the condition $\varepsilon_D \gg T_C$, has the form [13]

$$T_C = \frac{2\gamma}{\pi} \varepsilon_D \exp\left[-\frac{1}{U_0 N_F}\right], \quad (23)$$

where $\gamma = e^C$, $C \approx 0.577$ is the Euler's constant. In general case, the critical temperature is determined by zero of the function

$$\Psi_p\left(\frac{T}{\varepsilon_D}, \Gamma, g\right) \equiv 1 - \frac{g}{2} \int_{-\varepsilon_D/T}^{\varepsilon_D/T} \sqrt{1 + \frac{T}{\varepsilon_D} \Gamma y} \cdot \operatorname{th}\left(\frac{y}{2}\right) \frac{dy}{y}, \quad (24)$$

depending on the three dimensionless parameters T/ε_D , $\Gamma \equiv \varepsilon_D/\varepsilon_F$ and $g = U_0 N_F$. Dependence of the critical temperature on the parameter Γ at a fixed value of g is shown in figure 2. At maximum possible value $\Gamma = 1$, the critical temperature decreases by nearly 10%.

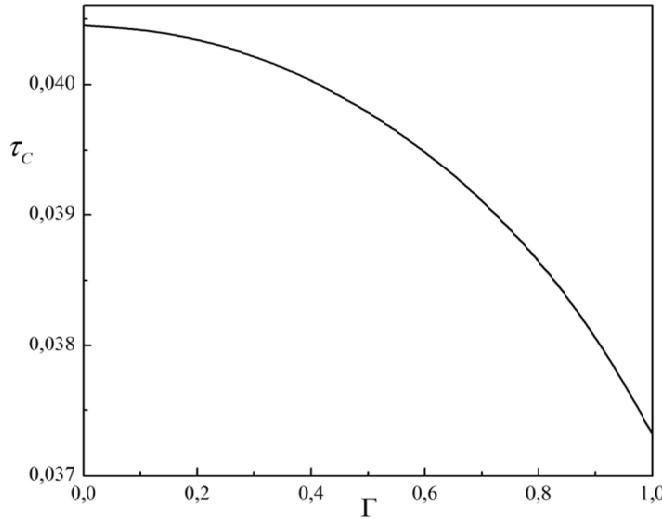


Fig. 2. Dependence of the critical temperature on the ratio of the Debye energy to the Fermi energy
 $\tau_c \equiv T_c/\varepsilon_D = \tau_c(\Gamma)$, $g = 0.3$

CRITICAL TEMPERATURE IN THE CASE OF THE DEGENERATE KERNEL

If the potential can be represented in the form

$$U(k, k') = - \sum_{i=1}^N \nu_i U_i(k) U_i(k'), \quad (25)$$

where $\nu_i = +1$ or $\nu_i = -1$ and N is a finite number, then the kernel in the integral equation (13):

$$K(k, k') = \sum_{i=1}^N \nu_i K_i(k) K_i(k'), \quad (26)$$

and besides

$$K_i(k) = U_i(k) \frac{k}{2\pi} \sqrt{F(k)}. \quad (27)$$

For such kernel (26), which is called degenerate, finding of the characteristic numbers λ or the corresponding

eigenvalues $\sigma \equiv 1/\lambda$ is reduced to finding of roots of the algebraic equation [17]

$$\Delta(\sigma) \equiv \begin{vmatrix} v_1 K_{11} - \sigma & v_2 K_{12} & \dots & v_N K_{1N} \\ v_1 K_{21} & v_2 K_{22} - \sigma & \dots & v_N K_{2N} \\ \dots & \dots & \dots & \dots \\ v_1 K_{N1} & v_2 K_{N2} & \dots & v_N K_{NN} - \sigma \end{vmatrix} = 0, \quad (28)$$

where

$$K_{ij} = K_{ji} \equiv \frac{1}{(2\pi)^2} \int_0^\infty U_i(k) U_j(k) F(k) k^2 dk. \quad (29)$$

It is obviously that $K_{ii} > 0$. As noted above, a phase transition occurs when, at decreasing temperature, one of the roots becomes unity in the transition point. If for a given potential that does not take place, then no phase transition exists.

Let's consider in more detail the simpler case $N = 2$, when the potential is represented in the form

$$U(k, k') = -v_1 U_1(k) U_1(k') - v_2 U_2(k) U_2(k'). \quad (30)$$

Then, according to (28), the characteristic numbers are determined from the quadric equation

$$\sigma^2 - \sigma(v_1 K_{11} + v_2 K_{22}) + v_1 v_2 (K_{11} K_{22} - K_{12}^2) = 0, \quad (31)$$

having the solutions

$$\sigma_{\pm} = \frac{1}{2} [(v_1 K_{11} + v_2 K_{22}) \pm D], \quad (32)$$

where $D = \sqrt{(v_1 K_{11} - v_2 K_{22})^2 + 4v_1 v_2 K_{12}^2}$. For solutions (32), there are obvious relations

$$\begin{aligned} \sigma_+ - \sigma_- &= D > 0, & \sigma_+ + \sigma_- &= v_1 K_{11} + v_2 K_{22}, \\ \sigma_+^2 - \sigma_-^2 &= (v_1 K_{11} + v_2 K_{22}) D, & \sigma_+ \sigma_- &= v_1 v_2 (K_{11} K_{22} - K_{12}^2), \end{aligned} \quad (33)$$

so that $\sigma_+ > \sigma_-$. Hence, if $v_1 K_{11} + v_2 K_{22} < 0$ and $v_1 v_2 (K_{11} K_{22} - K_{12}^2) > 0$, then both eigenvalues are negative and a phase transition into a superfluid state is not possible. Whereas if $v_1 K_{11} + v_2 K_{22} > 0$, then for $v_1 v_2 (K_{11} K_{22} - K_{12}^2) < 0$ one eigenvalue is positive $\sigma_+ > 0$ and another is negative $\sigma_- < 0$, and for $v_1 v_2 (K_{11} K_{22} - K_{12}^2) > 0$ both eigenvalues are positive. In both latter cases the critical temperature is determined by the condition $\lambda_+(T_C) = 1/\sigma_+(T_C) = 1$, so that the equation for T_C is the following

$$v_1 K_{11}(T_C) + v_2 K_{22}(T_C) + \sqrt{[v_1 K_{11}(T_C) - v_2 K_{22}(T_C)]^2 + 4v_1 v_2 K_{12}^2(T_C)} = 2. \quad (34)$$

This equation can be written as well in the form

$$[v_1 K_{11}(T_C) + v_2 K_{22}(T_C)] - v_1 v_2 [K_{11}(T_C) K_{22}(T_C) - K_{12}^2(T_C)] = 1. \quad (35)$$

As a concrete example, let's consider calculation of the critical temperature when, besides the attraction described by the BCS model, there is also repulsion in a certain shell around the Fermi surface. Then $v_1 = 1$, $v_2 = -1$ and $U_1(k) = \sqrt{U_0} \psi_1(k)$, $U_2(k) = \sqrt{U_C} \psi_2(k)$, and besides $\psi_1(k) = \theta(k - k_F - \Delta k_1) - \theta(k - k_F + \Delta k_1)$, $\psi_2(k) = \theta(k - k_F - \Delta k_2) - \theta(k - k_F + \Delta k_2)$, $\Delta k_1 = m_* \omega_D / \hbar k_F$, $\Delta k_2 = m_* \omega_C / \hbar k_F$. Here $\omega_C \approx \epsilon_F / \hbar$, so that $\Delta k_2 > \Delta k_1$. This model approximately describes the influence of the Coulomb repulsion on the superconducting transition temperature. From equation (35) it follows

$$K_{11}(T_C) = 1 + \frac{K_{12}^2(T_C)}{1 + K_{22}(T_C)}, \quad (36)$$

where in the present case

$$\begin{aligned} K_{11}(T_C) &= \sqrt{\frac{U_0}{U_C}} K_{12}(T_C) = \frac{U_0 N_F}{2} \int_{-\varepsilon_D/T_C}^{\varepsilon_D/T_C} \sqrt{1 + \frac{T_C}{\varepsilon_F}} y \cdot \operatorname{th}\left(\frac{y}{2}\right) \frac{dy}{y}, \\ K_{22}(T_C) &= \frac{U_C N_F}{2} \int_{-\varepsilon_F/T_C}^{\varepsilon_F/T_C} \sqrt{1 + \frac{T_C}{\varepsilon_F}} y \cdot \operatorname{th}\left(\frac{y}{2}\right) \frac{dy}{y}. \end{aligned} \quad (37)$$

As shown above, even for maximum $\Gamma \equiv \varepsilon_D/\varepsilon_F = 1$ at replacement of the root under integrals (37) by unity the difference from the exact result is no more than 10%. From this approximation it follows

$$K_{11} = g_0 \Theta, \quad K_{22} = g_C \left(\Theta + \ln \frac{\varepsilon_F}{\varepsilon_D} \right), \quad K_{12} = \sqrt{g_0 g_C} \Theta, \quad (38)$$

where $g_0 \equiv U_0 N_F$, $g_C \equiv U_C N_F$, $\Theta \equiv \ln \frac{2\gamma\varepsilon_D}{\pi T_C}$. Then from (36) the equation for the critical temperature follows

$$\Theta \left[g_0 - \frac{g_C}{1 + g_C \ln(\varepsilon_F/\varepsilon_D)} \right] = 1, \quad (39)$$

which coincides exactly with the one obtained in the model under discussion earlier [5,13]. Note, that in [13] it is stressed that the integral equation determining the critical temperature is very difficult to solve even for a simple interaction, and therefore the consideration carried out in [13] proves to be “quite approximate”. However, as shown above, formula (39) is exact for the selected model interaction.

CRITICAL TEMPERATURE FOR PAIR POTENTIALS OF GENERAL FORM

If we have such a potential that the kernel of integral equation (13) cannot be represented in the form of (16) or (26), then there exists an infinite number of characteristic numbers. In this case we have to employ approximate methods for finding characteristic numbers of the symmetric kernels [17-19]. Reasonably efficient is the Ritz method, and we will employ it for finding eigenvalues (characteristic numbers) of the non-degenerate kernels. Since in the problem under study eigenfunctions are defined on the half-axis $0 \leq k < \infty$, it is convenient to expand them in the functions $l_n(k/k_F) \equiv \exp(-k/2k_F) L_n(k/k_F)$, which are expressed through the Laguerre polynomials $L_n(k/k_F)$ [20]:

$$\Phi(k) = \sum_{n=0}^{\infty} B_n l_n(k/k_F). \quad (40)$$

Since the orthogonality relation holds for the introduced functions, $\int_0^{\infty} l_n(k) l_m(k) dk = \delta_{nm}$, then the coefficients of the expansion (40) are defined by formula

$$B_n = \frac{1}{k_F} \int_0^{\infty} \Phi(k) l_n(k/k_F) dk. \quad (41)$$

From the normalization condition it follows $\sum_{n=0}^{\infty} B_n^2 = 1$. Expansion (40) holds for functions satisfying the requirement of square integrability [20]:

$$\int_0^{\infty} \Phi^2(k) e^{-k/k_F} dk < \infty. \quad (42)$$

Then, the integral equation (13) is reduced to the system of an infinite number of homogeneous linear equations

$$\sum_{n=0}^{\infty} [\sigma \delta_{mn} - K_{mn}] B_n = 0, \quad (43)$$

where

$$K_{nm} = K_{mn} = -\frac{1}{(2\pi)^2} \int_0^{\infty} \int_0^{\infty} U(k, k') e^{-\frac{(k+k')}{2k_F}} L_n\left(\frac{k}{k_F}\right) L_m\left(\frac{k'}{k_F}\right) \sqrt{F(k) F(k')} kk' dk dk'. \quad (44)$$

The eigenvalues are determined by the condition of the determinant equaling zero

$$\det[\sigma \delta_{mn} - K_{mn}] = 0. \quad (45)$$

In the Ritz method the infinite determinant is replaced by the determinant of the finite matrix. Since a phase transition takes place under satisfaction of the condition $\sigma(T_C) = \lambda^{-1}(T_C) = 1$, then the equation for the critical temperature of a phase transition takes the form

$$\det[\delta_{mn} - K_{mn}(T_C)] = 0. \quad (46)$$

If in expansion (40) only two main terms with $n = 0$ and $n = 1$ are left, then from (45) it follows the quadratic equation for approximate determination of the two highest by absolute value eigenvalues

$$\sigma^2 - \sigma(K_{00} + K_{11}) + K_{00}K_{11} - K_{01}^2 = 0. \quad (47)$$

Hence

$$\sigma_{\pm} = \frac{1}{2}(K_{00} + K_{11} \pm D), \quad (48)$$

where $D = \sqrt{(K_{00} - K_{11})^2 + 4K_{01}^2}$. From obvious relations for solutions (48)

$$\begin{aligned} \sigma_+ - \sigma_- &= D > 0, & \sigma_+ + \sigma_- &= K_{00} + K_{11}, \\ \sigma_+^2 - \sigma_-^2 &= (K_{00} + K_{11})D, & \sigma_+\sigma_- &= K_{00}K_{11} - K_{01}^2 \end{aligned} \quad (49)$$

it follows that, if $K_{00} + K_{11} < 0$ and $K_{00}K_{11} - K_{01}^2 > 0$, then both roots (48) are negative and a phase transition is absent.

Whereas if $K_{00} + K_{11} > 0$, then one (for $K_{00}K_{11} - K_{01}^2 < 0$) or two (for $K_{00}K_{11} - K_{01}^2 > 0$) positive roots exist, and the transition temperature is determined from the condition $\sigma_+(T_C) = 1$, so that

$$K_{00}(T_C) + K_{11}(T_C) + \sqrt{[K_{00}(T_C) - K_{11}(T_C)]^2 + 4K_{01}^2(T_C)} = 2, \quad (50)$$

or

$$[K_{00}(T_C) + K_{11}(T_C)] - [K_{00}(T_C)K_{11}(T_C) - K_{01}^2(T_C)] = 1. \quad (51)$$

Consider one more method of approximate determination of the critical temperature not requiring use of the eigenfunctions. For a symmetric kernel under the normalization condition $\int_0^\infty \Phi_i(k)\Phi_j(k)dk = \delta_{ij}$ the bilinear expansion holds [15]:

$$K(k, k') = \sum_{j=1}^N \frac{\Phi_j(k)\Phi_j(k')}{\lambda_j}. \quad (52)$$

Here the number of characteristic numbers N can be finite for degenerate kernels and infinite in general case. It is assumed that the following conditions are satisfied for the kernel

$$\int_0^\infty K(k, k'; T_C)dkdk' < +\infty, \quad \int_0^\infty K^2(k, k'; T_C)dkdk' < +\infty, \quad (53)$$

i.e. the integral equation is of Fredholm type. If kernel (52) is continuous and its characteristic numbers are all positive, or there is only a finite number of negative characteristic numbers, then the bilinear series of this kernel converges uniformly (Mercer's theorem) [15,17]. Assuming in (52) $k = k'$ and integrating both sides by k , we obtain the formula for the trace of the continuous kernel $K(k, k')$

$$\int_0^\infty K(k, k)dk = \sum_{i=1}^N \frac{1}{\lambda_i}. \quad (54)$$

Squaring both sides of equation (52) and integrating by k and k' , we come as well to the relation

$$\int_0^\infty \int_0^\infty K^2(k, k')dkdk' = \sum_{j=1}^N \frac{1}{\lambda_j^2}. \quad (55)$$

Taking into account that $\lambda_1(T_C) = 1$ in the transition point, formulae (54) and (55) can be used for both an approximate calculation of the critical temperature and checking self-consistency of calculations of the critical temperature by other approximate methods. If the maximum eigenvalue $\sigma_1 = 1/\lambda_1$ is positive and $\sigma_1 \gg |\sigma_2| > |\sigma_3| > \dots$, then the equation

$$\int_0^\infty K(k, k; T_C)dk = 1, \quad (56)$$

following from (54), can be used for calculation of T_C . However, this approximation is by no means always valid. It can turn out that, in addition to the maximum positive eigenvalue, a substantial contribution is made by another eigenvalue which, if negative, can even exceed by absolute value a contribution of the positive eigenvalue. Therefore, for obtaining more accurate equation for T_C , at least the two maximum by absolute value eigenvalues σ_1 and σ_2 should be taken into account. From (54) and (55), the system of algebraic equations follows for these eigenvalues

$$\sigma_1 + \sigma_2 = K_1 \equiv \int_0^\infty K(k, k) dk = -\frac{1}{(2\pi)^2} \int_0^\infty U(k, k) F(k) k^2 dk, \quad (57)$$

$$\sigma_1^2 + \sigma_2^2 = K_2 \equiv \int_0^\infty \int_0^\infty K^2(k, k') dk dk' = \frac{1}{(2\pi)^4} \int_0^\infty \int_0^\infty U^2(k, k') F(k) F(k') k^2 k'^2 dk dk'. \quad (58)$$

The solutions of this system of equations are:

$$\sigma_{1,2} = \frac{1}{2}(K_1 \pm D), \quad (59)$$

where $D = \sqrt{2K_2 - K_1^2}$. Here the subradical expression $2K_2 - K_1^2 > 0$, because all characteristic numbers of an integral equation with a symmetric kernel are real. The obvious relations hold

$$\sigma_1 - \sigma_2 = D, \quad \sigma_1^2 - \sigma_2^2 = K_1 D, \quad \sigma_1 \sigma_2 = \frac{1}{2}(K_1^2 - K_2). \quad (60)$$

If $K_1 < -D$ and $K_1^2 > K_2$, then both roots are negative and a phase transition is absent. If $K_1 > -D$ and $K_1^2 - K_2 < 0$, then $\sigma_1 > 0$ and $\sigma_2 < 0$, and besides, if in this case $K_1 < 0$, then $|\sigma_2| > \sigma_1$. If $K_1 > -D$ and $K_1^2 - K_2 > 0$, then both roots are positive and $\sigma_1 > \sigma_2$. Thus, with account of the two characteristic numbers the equation for the critical temperature has the form

$$K_1(T_C) + \sqrt{2K_2(T_C) - K_1^2(T_C)} = 2, \quad (61)$$

or, equivalently,

$$K_1(T_C) = 1 \pm \sqrt{K_2(T_C) - 1}. \quad (62)$$

In the latter formula the plus sign should be taken if $K_1^2 - K_2 > 0$, and the minus sign if $K_1^2 - K_2 < 0$.

For estimation of value of the minimum (by absolute value) characteristic number $\lambda_i(T_C)$ ($i \neq 1$), the method of iterated kernels [15,17,19] can be used, for instance. The iterated kernel is defined by the relation

$$K_m(k, k') \equiv \int_0^\infty K(k, k_1) K(k_1, k_2) \dots K(k_{m-1}, k') dk_1 dk_2 \dots dk_{m-1}, \quad (63)$$

and its trace by the relation

$$S_m \equiv \int_0^\infty K_m(k, k) dk = \sum_{i=1}^N \frac{1}{\lambda_i^m}. \quad (64)$$

In the transition point

$$S_m(T_C) \equiv \int_0^\infty K_m(k, k; T_C) dk = 1 + \sum_{i=2}^N \frac{1}{\lambda_i^m(T_C)}. \quad (65)$$

Formula (65) enables to estimate the value of the minimum different from unity characteristic number $|\lambda_2(T_C)|$. If $|\lambda_2(T_C)| > 1$, then

$$|\lambda_2(T_C)| = \left[|S_m(T_C) - 1| \right]^{-1/m}. \quad (66)$$

And if $|\lambda_2(T_C)| < 1$, then

$$|\lambda_2(T_C)| = \left[|S_m(T_C)| \right]^{-1/m}. \quad (67)$$

Formulae (66), (67) can be used for checking self-consistency of calculation of the critical temperature by approximate methods.

TEMPERATURE OF TRANSITION INTO HELIUM-3 SUPERFLUID PHASE FOR THE MORSE POTENTIAL

Now we apply the proposed calculation methods to evaluate the critical temperature of the superfluid transition of liquid ${}^3\text{He}$ into p -wave ($l=1$) pairing state, using the known Morse potential

$$U(r) = u_0 \left\{ \exp[-2(r - r_0)/L] - 2 \exp[-(r - r_0)/L] \right\}, \quad (68)$$

which is widely used for modeling of interactions between atoms and has the three parameters u_0 , r_0 , L . The parameters r_0 and u_0 define the minimum point of the potential (a distance between atoms and a depth of the potential well in this point) and the parameter L characterizes a scale of potential variation. Fourier component of potential (68) has the form

$$U_1(k, k') = \frac{\pi u_0 L^3}{2} \left[\exp\left(\frac{2r_0}{L}\right) I\left(\frac{kL}{2}, \frac{k'L}{2}\right) - 16 \exp\left(\frac{r_0}{L}\right) I(kL, k'L) \right], \quad (69)$$

where

$$I(x, y) \equiv \frac{(1+x^2+y^2)}{xy \left[1+(x-y)^2 \right] \left[1+(x+y)^2 \right]} - \frac{1}{4x^2y^2} \ln \frac{1+(x+y)^2}{1+(x-y)^2}. \quad (70)$$

In this case the kernel

$$K(k, k') = -\frac{u_0 L^3}{8\pi} \left[\exp\left(\frac{2r_0}{L}\right) I\left(\frac{kL}{2}, \frac{k'L}{2}\right) - 16 \exp\left(\frac{r_0}{L}\right) I(kL, k'L) \right] kk' \sqrt{F(k)F(k')} \quad (71)$$

is not degenerate and approximate methods should be used for calculation of the critical temperature.

For numerical calculation of the ${}^3\text{He}$ superfluid transition the following values of the potential parameters are used: $r_0 = 2.95 \cdot 10^{-8} \text{ cm}$, $u_0 / k_B = 10.0 \text{ K}$. The parameter L is chosen from such a criterion that the calculated scattering length

$$a_0 = \frac{m}{4\pi\hbar^2} \int U(r) d\mathbf{r} = \frac{u_0 m}{4\hbar^2} L^3 e^{\frac{r_0}{L}} \left(e^{\frac{r_0}{L}} - 16 \right) \quad (72)$$

should be close to the average adopted in the literature value $a_0 = -8.2 \text{ \AA}$ [21]. It gives for the dimensionless parameter $\tilde{L} \equiv L/r_0$ the value $\tilde{L} = 0.386$. The following parameters of the liquid helium are chosen: the density of atoms $n = 1.8 \cdot 10^{22} \text{ cm}^{-3}$, that corresponds to the mass density $\rho_m = 0.08 \text{ g} \cdot \text{cm}^{-3}$, the Fermi wave number and the Fermi temperature $k_F = 0.81 \cdot 10^8 \text{ cm}^{-1}$, $T_F = 1.71 \text{ K}$. Numerical calculation by the Ritz method in the approximation of two characteristic numbers gives the value $\tau_c = 6.604 \cdot 10^{-4}$, that corresponds to the critical temperature $T_c \approx 1.1 \text{ mK}$. Note that experimentally observable transition temperature increases from the value $T_c \approx 0.9 \text{ mK}$ at zero pressure to the value $T_c \approx 2.6 \text{ mK}$ at the maximum possible pressure [11]. Calculation by formula (48) of the second eigenvalue gives the value $\sigma_-(\tau_c) = -12.8$. In order to check self-consistency of the result obtained above by the Ritz method, let's compare the value of the characteristic number $\lambda_-(\tau_c) = \sigma_-(\tau_c)^{-1} = -0.078$ with the value of this number calculated independently by the trace method (67). Result of calculation by the trace method converges rather rapidly with increasing a number of iterations m , and for $m = 3$ gives the value $\lambda_-^{(3)}(\tau_c) \approx -0.082$. This result differs from that one obtained above by the Ritz method by nearly 5%, that indicates good accuracy of this approximation with regard to the Morse potential.

Let's calculate the critical temperature of the phase transition by another method based on using the relations (54), (55) with account of two eigenvalues that leads to equations (61), (62). For the same set of parameters of the system and the potential as that used above, we get $\tau_c = 1.43 \cdot 10^{-2}$ and $T_c \approx 24.5 \text{ mK}$. The second eigenvalue, obtained by formula (59), $\sigma_2(\tau_c) = -16.4$ and the corresponding characteristic number $\lambda_2(\tau_c) = \sigma_2(\tau_c)^{-1} = -0.061$. Calculation by the trace method gives $\lambda_2^{(3)}(\tau_c) \approx -0.077$ for $m = 3$. In this case the characteristic numbers obtained by different ways differ by nearly 20%. Therefore, the second method gives a less accurate result than the Ritz method and leads to the overestimated value of the superfluid transition temperature.

It should be noted that the value of the critical temperature proves to be very sensitive the value of the dimensionless parameter \tilde{L} . As shown in table 1, variation of this parameter by only 0.001 ($\approx 0.25\%$) leads to variation of the critical temperature by two-three times. Such strong dependence can be connected with the fact that the parameter \tilde{L} of the Morse potential defines the relation between quantities of the attractive and the repulsive parts of the potential. With increasing \tilde{L} the role of the repulsive part of the potential falls and of the attractive part rises exponentially, and this presumably causes high sensitivity of the transition temperature to this parameter.

Table 1.

Dependence of the critical temperature and the scattering length on the parameter $\tilde{L} = L/r_0$ of the Morse potential

\tilde{L}	0.385	0.386	0.387
$T_c \text{ mK}$	0.35	1.1	2.3
$a_0 \text{ \AA}$	-7.9	-8.2	-8.5

CONCLUSIONS

A method for calculation of the temperature of a phase transition of a many-particle Fermi system into a superfluid or a superconducting state, based on transition to a homogeneous integral equation with a symmetric kernel, is

proposed. For potentials bringing to a degenerate kernel of an integral equation the problem of determination of the critical temperature is solvable exactly, and for potentials of general form approximate methods of finding eigenvalues of homogeneous integral equations with symmetric kernels can be employed. The developed method enables to calculate the temperature of transition into the superfluid state for an arbitrary pair potential with a desired accuracy. As examples of use of the method, the results of the BCS model with account of a finite ratio of the Debye energy to the Fermi energy are reproduced and the influence of the Coulomb interaction on the critical temperature is analyzed. It is shown that the known formula [5,13] for the critical temperature in the BCS model accounting for the Coulomb interaction is exact for the selected model. The temperature of the superfluid transition of liquid ^3He into p -wave pairing state for the Morse potential is calculated. It is shown that the calculated temperature depends strongly on the value of one of parameters of the potential and at reasonable choice of parameters calculation gives the value of the critical temperature close to the experimentally observable one. The developed method of calculation can be employed for determination of temperatures of phase transitions in other physical systems.

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